1-Nitrobutane

627-05-4 | DTXSID8020967

Model Performance

Model	Data
IVIOGEI	Dala

Weighted KNN model

5-fold CV (75%)		Training	Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.89	0.25	0.88	0.26	0.75	0.38	

Model Results

Predicted value: 4.46 days

Global applicability domain: Outside

Local applicability domain index: 2.86e-01

Confidence level: 7.64e-01

Nearest Neighbors from the Training Set

Image not found
2-Methylhexane
Measured: 3.00
Predicted: 5.54

Image not found
Tetradeca-1,13-diene
Measured: 13.0
Predicted: 8.69

Image not found
2-Methylheptane
Measured: 3.00
Predicted: 3.99